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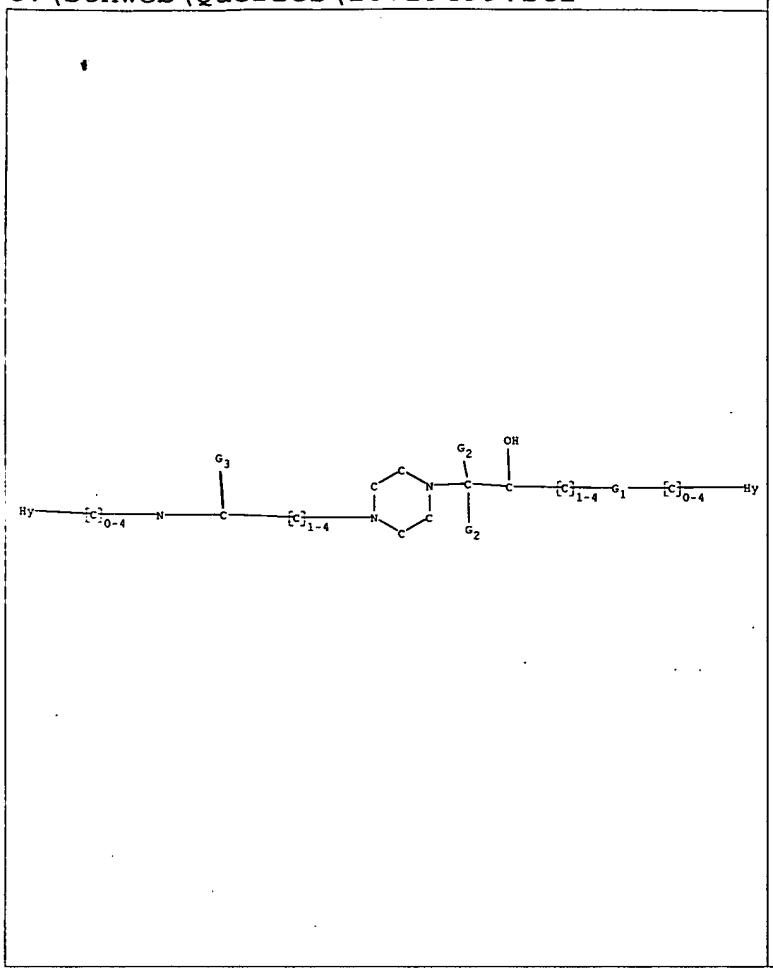

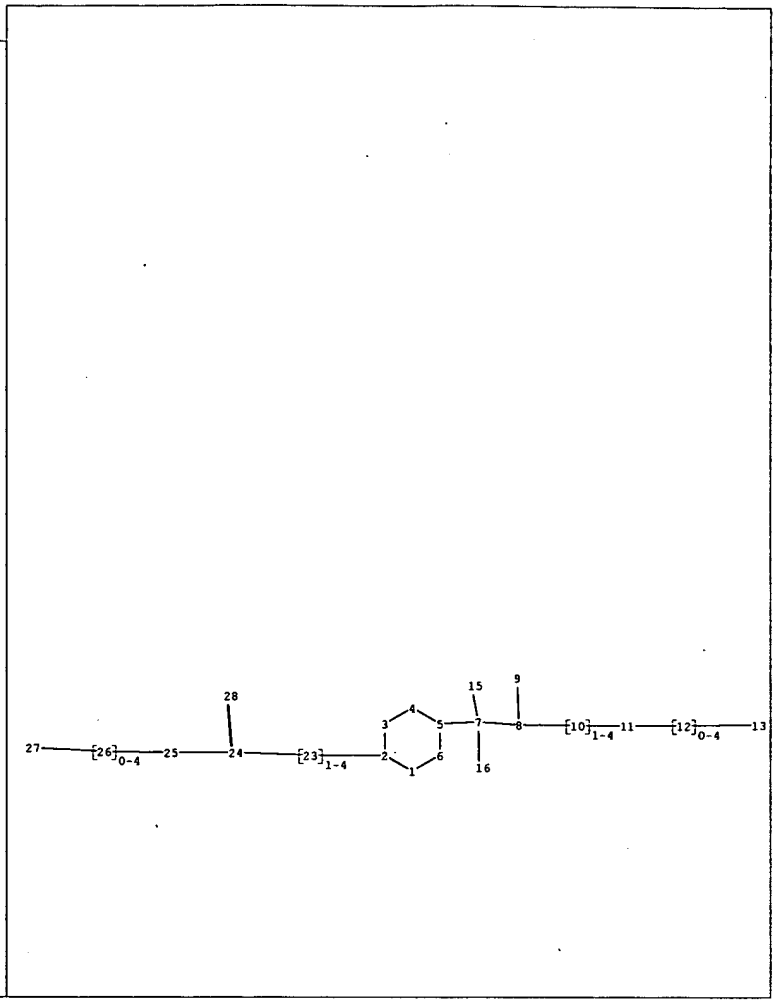

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ring nodes :
1 2 3 4 5 6
chain bonds :
2-23 5-7 7-8 7-15 7-16 8-9 8-10 10-11 11-12 12-13 23-24 24-25
24-28 25-26 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 2-23 3-4 4-5 5-6 5-7 7-15 7-16 8-9 10-11 11-12
12-13 24-25 24-28 25-26 26-27
exact bonds :
7-8 8-10 23-24
isolated ring systems :
containing 1 :

G1:O,S,N

G2:H,CH3

G3:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:Atom 15:CLASS 16:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:Atom 28:CLASS
Generic attributes :

13:
Saturation : Unsaturated
27:
Saturation : Unsaturated

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Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading structure

L7      STRUCTURE UPLOADED

=> s l7
SAMPLE SEARCH INITIATED 11:33:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      243 TO ITERATE

100.0% PROCESSED      243 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         3925 TO     5795
PROJECTED ANSWERS:               0 TO        0

L8             0 SEA SSS SAM L7

=> s l7 sss full
FULL SEARCH INITIATED 11:35:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     5026 TO ITERATE

100.0% PROCESSED     5026 ITERATIONS                               12 ANSWERS
SEARCH TIME: 00.00.01

L9            12 SEA SSS FUL L7

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COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 167.35     346.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00      -0.73

FILE 'CAPLUS' ENTERED AT 11:35:45 ON 02 OCT 2005
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FILE COVERS 1907 - 2 Oct 2005  VOL 143 ISS 15
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FILE LAST UPDATED: 30 Sep 2005  (20050930/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

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L10           3 L9

=> d l10 1-3 bib abs hitstr

L10  ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2005 ACS on STN
Full Text
AN   2004:515509  CAPLUS
DN   141:71566
TI   Preparation of hydroxybenzothiazolyloxypropylpiperazines as fatty acid
     oxidation inhibitors.
IN   Elzein, Elfatih; Koltun, Dmitry; Zablocki, Jeff
PA   CV Therapeutics, Inc., USA
SO   PCT Int. Appl., 68 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     WO 2004052887         A3    20040715
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2508608            AA    20040624    CA 2003-2508608         20031205
     US 2004152890         A1    20040805    US 2003-729499          20031205
     EP 1567525            A2    20050831    EP 2003-812835          20031205
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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OS   MARPAT 141:71566
GI
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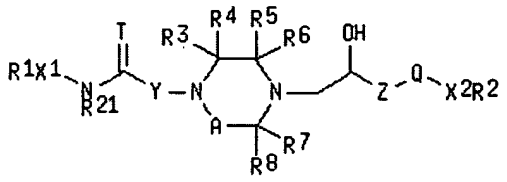
Apps



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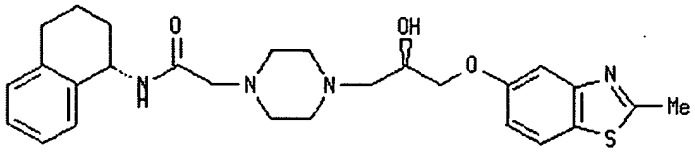


II

AB Title compds. [I; R1, R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, heteroaryl; X1 = bond, (CR15R16)p; X2 = bond, (CR18R19)q; R15, R16 = H, OH, alkyl, CO2R17; R17 = H, alkyl, (substituted) Ph; n, p, q = 1-3; R21 = H, alkyl; T = O, S; Y, Z = (CR18R19)q; R11, R12, r13, R14, R18, R19 = H, alkyl; A = (CR9R10)m; m = 1, 2; R3-R10 = H, alkyl, COR; R = OR11, NR11R12; R3R4, R5R6, R7R8, R9R10 = O; R3R7, R3R9, R5R7, R5R9 = (CR13R14)n; Q = O, S, NR20; R20 = H, (substituted) alkyl; with provisos], were claimed. Title compd. (II) inhibited palmitoyl CoA oxidn. with IC50 = 0.08 μM.

IT **678982-07-5P 678982-12-2P 709041-43-0P 709041-44-1P 709041-45-2P**

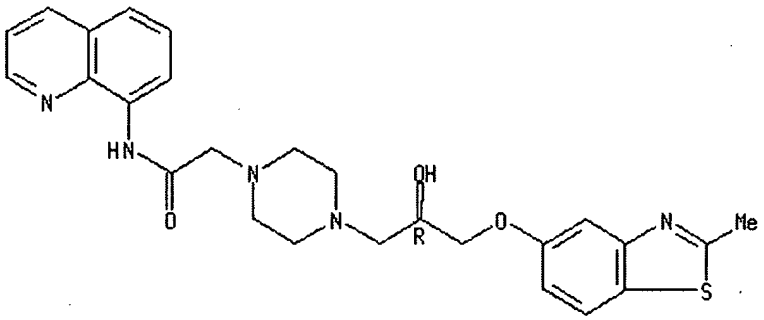
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compd.; prepn. of hydroxybenzothiazolyloxypropylpiperazines as fatty acid oxidn. inhibitors)

RN 678982-07-5 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-8-quinolinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

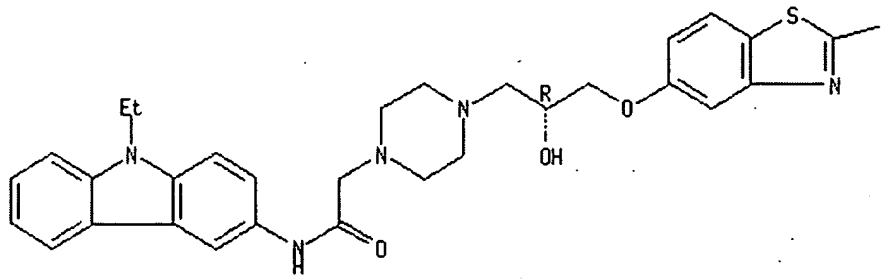


RN 678982-12-2 CAPLUS

CN 1-Piperazineacetamide, N-(9-ethyl-9H-carbazol-3-yl)-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



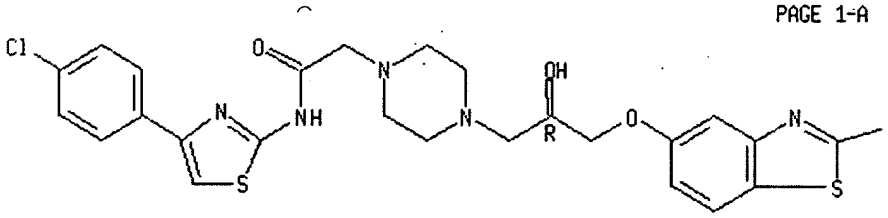
PAGE 1-B

Me

RN 709041-43-0 CAPLUS
CN 1-Piperazineacetamide, N-[4-(4-chlorophenyl)-2-thiazolyl]-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



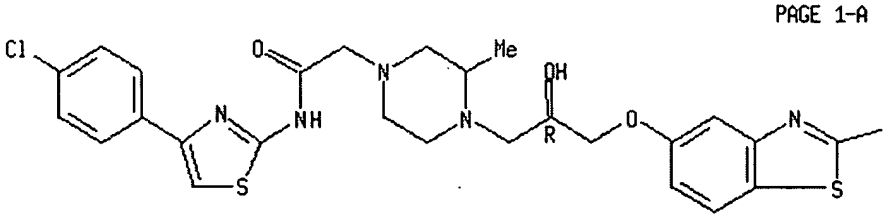
PAGE 1-B

Me

RN 709041-44-1 CAPLUS
CN 1-Piperazineacetamide, N-[4-(4-chlorophenyl)-2-thiazolyl]-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

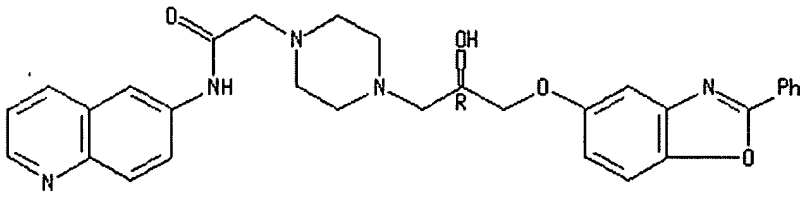


PAGE 1-B

—Me

RN 709041-45-2 CAPLUS
CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-phenyl-5-benzoxazolyl)oxy]propyl]-N-6-quinolinyl- (9CI) (CA INDEX NAME)

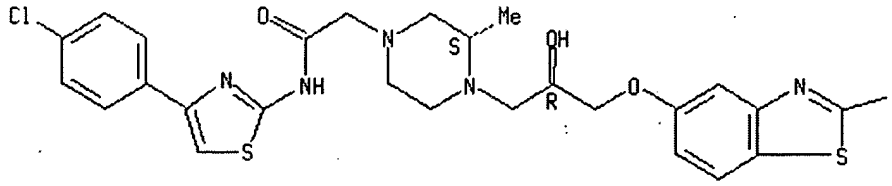
Absolute stereochemistry.



IT **709041-49-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of hydroxybenzothiazolyloxypropylpiperazines as fatty acid oxidn. inhibitors)
RN 709041-49-6 CAPLUS
CN 1-Piperazineacetamide, N-[4-(4-chlorophenyl)-2-thiazolyl]-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-3-methyl-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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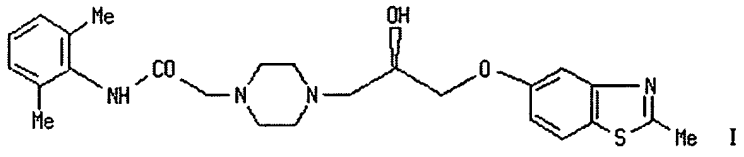
L10 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
Full Text
AN 2003:1002009 CAPLUS
DN 140:331785
TI New fatty acid oxidation inhibitors with increased potency lacking adverse metabolic and electrophysiological properties
AU Koltun, Dmitry O.; Marquart, Timothy A.; Shenk, Kevin D.; Elzein, Elfatih;

Li, Yuan; Nguyen, Marie; Kerwar, Suresh; Zeng, Dewan; Chu, Nancy; Soohoo, Daniel; Hao, Jia; Maydanik, Victoria Y.; Lustig, David A.; Ng, Khing-Jow; Fraser, Heather; Zablocki, Jeffery A.
CS Department of Bioorganic Chemistry, Palo Alto, CA, 94304, USA
SO Bioorganic Medicinal Chemistry Letters (2004), 14(2), 549-552
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
GI



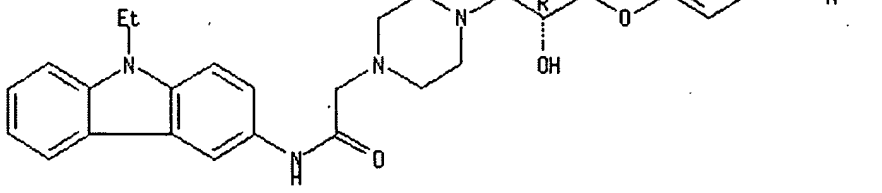
I

AB New inhibitors of palmitoylCoA oxidn. were synthesized based on a structurally novel lead, CVT-3501 (I). Investigation of structure-activity relationships was conducted with respect to potency of inhibition of cardiac mitochondrial palmitoylCoA oxidn. and metabolic stability. Three potent and metabolically stable analogs were evaluated in vitro for cytochrome P 450 inhibition and potentially adverse electrophysiol. effects. One compd. (II) was also found to have favorable pharmacokinetic properties in rat.

IT **678982-12-2P**
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(fatty acid oxidn. inhibitors with increased potency lacking adverse metabolic and electrophysiol. properties)
RN 678982-12-2 CAPLUS
CN 1-Piperazineacetamide, N-(9-ethyl-9H-carbazol-3-yl)-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

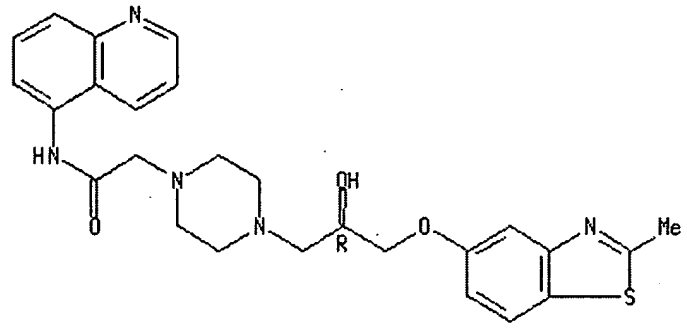
Me

IT **678982-06-4P 678982-07-5P 678982-08-6P**

678982-09-7P 678982-10-0P 678982-11-1P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(fatty acid oxidn. inhibitors with increased potency lacking adverse metabolic and electrophysiol. properties)

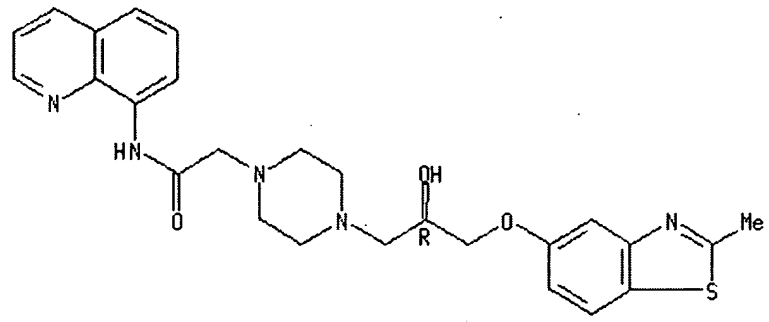
RN 678982-06-4 CAPLUS
CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-5-quinolinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



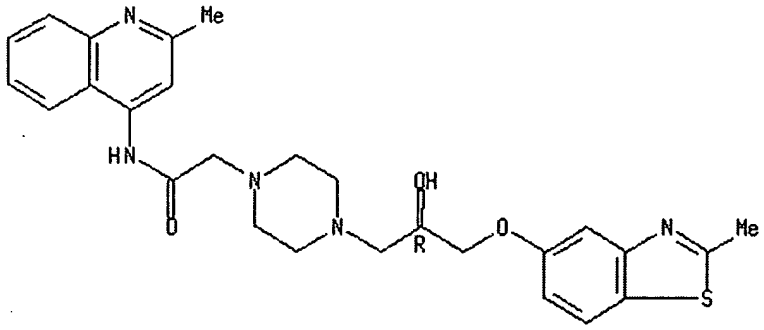
RN 678982-07-5 CAPLUS
CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-8-quinolinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



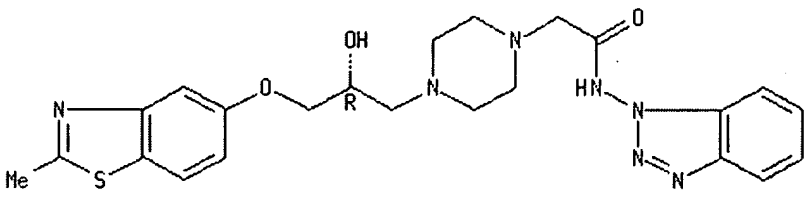
RN 678982-08-6 CAPLUS
CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-(2-methyl-4-quinolinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



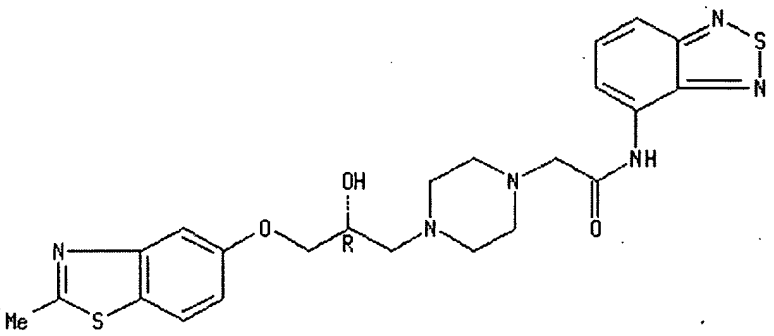
RN 678982-09-7 CAPLUS
CN 1-Piperazineacetamide, N-1H-benzotriazol-1-yl-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



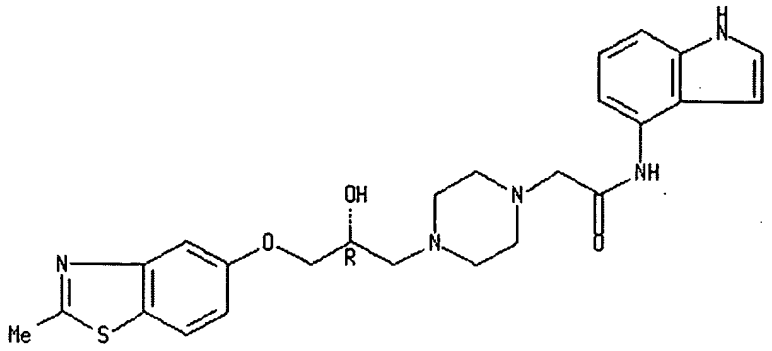
RN 678982-10-0 CAPLUS
CN 1-Piperazineacetamide, N-2,1,3-benzothiadiazol-4-yl-4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 678982-11-1 CAPLUS
CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-[(2-methyl-5-benzothiazolyl)oxy]propyl]-N-1H-indol-4-yl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
Full Text
AN 2002:314915 CAPLUS
DN 136:340700
TI Preparation of 4-[3-heteroaryloxy-2-hydroxypropyl]-1-piperazineacetamides as P-glycoprotein and/or MRP1 inhibitors for treating multidrug resistance
IN Degenhardt, Charles Raymond; Eickhoff, David Joseph
PA The Procter Gamble Company, USA
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 4

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OS MARPAT 136:340700
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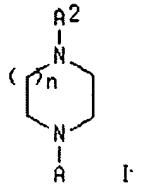

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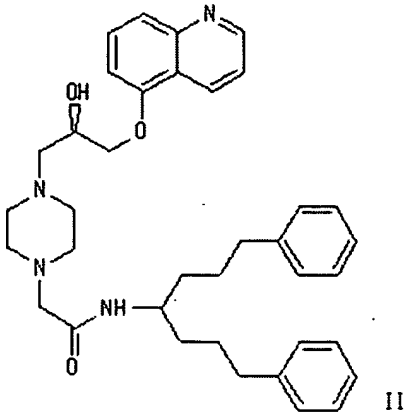


II

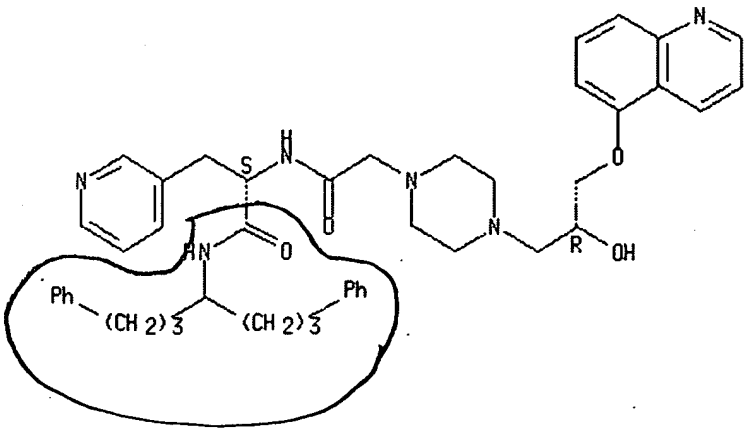
AB Title compds. I [wherein n = 1-3; A = A1 or A3; A1 = (CR1R1)xD1OyD2zR2; R1 = independently H, OH, (un)substituted hydrocarbon, heterogeneous group, carboxylic group, heterocyclic, or (hetero)arom.; x = 0-10; R2 = (un)substituted hydrocarbon, heterogeneous group, carboxylic group, heterocyclic, or (hetero)arom.; D1 and D2 = independently CO or NR3; R3 = H or R2; or R2R3 may form a heterocycle; y = 0-1 and z = 0-1 with provisos; A2 = (CR1R1)uD3(CR1R1)pOvR5; u = 0-10; p= 0-10; v = 0-1; D3 = SO2, CO, or CR1OH with provisos; R5 = substituted hydrocarbon or heterogeneous group; A3 = D4(CR1R1)tD5; t = 1-6; D4 = CO or CHR1; D5 = NR6R7, OrR6, or COR6; r = 0-1; R6 = (un)substituted hydrocarbon, heterogeneous group, carboxylic group, heterocyclic, or (hetero)arom.; R7 = H or R6 with provisos; or optical isomers, diastereomers, enantiomers, pharmaceutically acceptable salts, or biohydrolyzable amides, esters, or imides thereof] were prepd. as P-glycoprotein and/or MRP1 inhibitors for treating multidrug resistance. For example, lithium 4-(tert-butoxycarbonyl)-1-(carboxymethyl)piperazine (prepn. given) was amidated with 1,7-diphenyl-4-heptylamine•HCl in the presence of 1-hydroxybenzotriazole, N,N-diisopropylethylamine, and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide in DMF. Deprotection and addn. of (R)-5-oxiranylmethoxyquinoline afforded II. The latter exhibited an accumulation index (ratio of fluorescence in the presence of modulator to fluorescence in the absence of modulator) of 10 in NIH-MDR1-G185 cells. I are useful as cancer therapeutic agents, antibacterial agents, antiviral agents, and antifungal agents (no data). Compns. of the substituted heterocyclic compds. are also disclosed.

IT **416857-33-5P**, N-[1-[2-(R)-Hydroxy-3-(quinolin-5-yloxy)propyl]piperazine-4-acetyl]-3-(3-pyridyl)alanine [4-phenyl-1-(3-phenylpropyl)butyl]amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Pgp and/or MRP1 inhibitor; prepn. of heteroaryloxyhydroxypropyl piperazineacetamides as P-glycoprotein or MRP1 inhibitors for treating multidrug resistance)

RN 416857-33-5 CAPLUS

CN 1-Piperazineacetamide, 4-[(2R)-2-hydroxy-3-(5-quinolinyloxy)propyl]-N-[(1S)-2-oxo-2-[[4-phenyl-1-(3-phenylpropyl)butyl]amino]-1-(3-pyridinylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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